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Mr Downing,

Attached is the missing page (page 3)
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Yvonne
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Memorandum to: Ms. Tammy Besecker

From: Deborah A. Levin

Subject: Report for AFOSR Project Ended Calendar Year 2002

Date: February, 24, 2003 *Grant, F49620-02-1-0104*

This memo is in response to a request from AFOSR for a final report due at the end of 2002. This material was provided to the project manager Dr. Mitat Birkan at his contractor's meeting of August 2002. It comprises the project final report and is presented again here. Please forward it to John McKee and any other appropriate people.

A main task completed under this project was to understand the sensitivity of chemical models used in the Direct Simulation Monte Carlo method to the pair selection techniques as well as the use of discrete versus continuum energy levels. The results are separated into three groups:

1. The impact of the parameters in the Arrhenius fit (A , B , E_a),

$$k(T) = AT^B \exp -E_a/kT$$

on the difference between the rate constant determined by the original Arrhenius fit and that produced using the TCE reaction probabilities with the discrete internal energies (uncorrected and corrected) was examined.

The impact was investigated for the reaction $\text{H}_2\text{O} + \text{O} \rightarrow \text{OH}(A) + \text{OH}(X)$, for which $A = 3.8 \times 10^{-21} \text{ m}^3/\text{s}$, $B = 1.3$, $E_a = 7.69 \times 10^{-19} \text{ J}$.

First, the parameter A does not effect the difference between the uncorrected reaction rate and the Arrhenius values.

Parameter B visibly impacts the difference. The more B differs from 0, the more the difference. This is shown in Fig. 1.

The influence of the reaction threshold, E_a , is even more pronounced. This is illustrated in Fig. 2.

We can therefore say that the uncorrected rate leads to larger errors for larger slope of the reaction rate constant as function of temperature.

Comparison of different reactants for same reaction rate constant ($A = 3.8 \times 10^{-21} \text{ m}^3/\text{s}$, $B = 1.3$, $E_a = 7.69 \times 10^{-19} \text{ J}$) shows that for larger number of internal degrees of freedom of reactants the difference is generally somewhat larger (even though the impact is smaller than for E_a). This is shown in Fig. 3.

The accuracy of the correction routine was checked for several values of E_a and fixed A and B (reaction $\text{H}_2\text{O} + \text{O} \rightarrow \text{OH}(A) + \text{OH}(X)$). It is seen that the correction enables one to quite accurately reconstruct the reaction rate constant given by the Arrhenius fit (see Figs.4-6).

2. Next part is related to the simulation of the flow about a rocket forebody at 50 km and velocity of 5 km/s. The main goal here was to see the impact of the reaction rate correction of the formation of OH. There are two major processes included: water dissociation by air species and exchange reaction between water and atomic oxygen.

General structure of the flow is shown in Figs. 7 and 8. The important issue is the molecular oxygen dissociation. It is seen from Fig. 9 that the molecular oxygen dissociates strongly in the shock, and there is much more atomic oxygen than O_2 .

The comparison of H_2O translational, vibrational, and overall temperature profiles along the stagnation line (body is at $X = 0$) is shown in Fig. 10. The most important parameter in terms of reactions is the overall temperature, since the TCE model is used here. The overall temperature in the shock layer is about 5500 K.

For this temperature regime (see also previous figure), the most important reaction is the exchange reaction between H_2O and O , as it is seen from the comparison of the rates of different OH formation mechanisms shown in Fig. 11. The exchange reaction is determined by $A = 1.13 \times 10^{-16} \text{ m}^3/\text{s}$, $B = 0$, $E_a = 4.818 \times 10^{-20} \text{ J}$. For this reaction which rate changes

very slowly with temperature the uncorrected reaction rate is very close to the corrected one. Therefore, we can expect results that are very close for the discrete corrected and uncorrected models.

This is exactly what was observed. The comparison of the number density profiles of H_2O and OH along the stagnation line for the discrete corrected and uncorrected models and the conventional continuum model is shown in Figs 12 and 13.

3. The third topic is modeling of two counter plumes. One consists of pure H_2O , and the other consists of pure O . The velocity of the plumes was chosen to be 5.5 km/s. The total relative speed is therefore 11 km/s, similar to the MirEx conditions.

Two reactions were considered,



and



The computation were performed separately for these processes to exclude their interference.

Again, three models were used: continuum and discrete with and without reaction rate correction. The general flowfield structure is shown in Fig. 14 and 15.

Comparison of the profiles of $OH(X)$ (reaction (1)) and $OH(A)$ (reaction (2)) number density along the stagnation line shows that the discrete corrected model and the continuum model produce similar results (this is in fact what was expected), whereas the uncorrected discrete model significantly underpredicts the production rate of both $OH(X)$ and $OH(A)$.

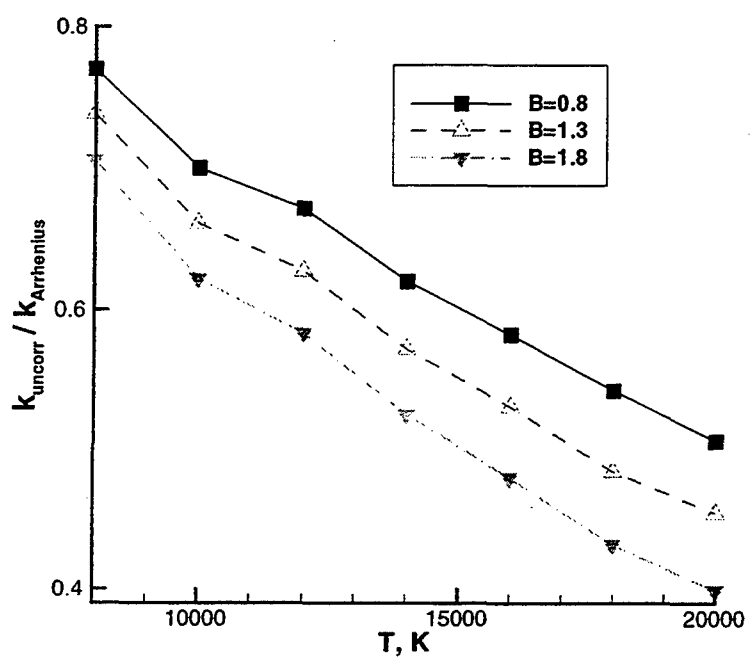


Figure 1: The impact of the parameter B in the Arrhenius fit on the ratio of the uncorrected to original reaction rate constants.

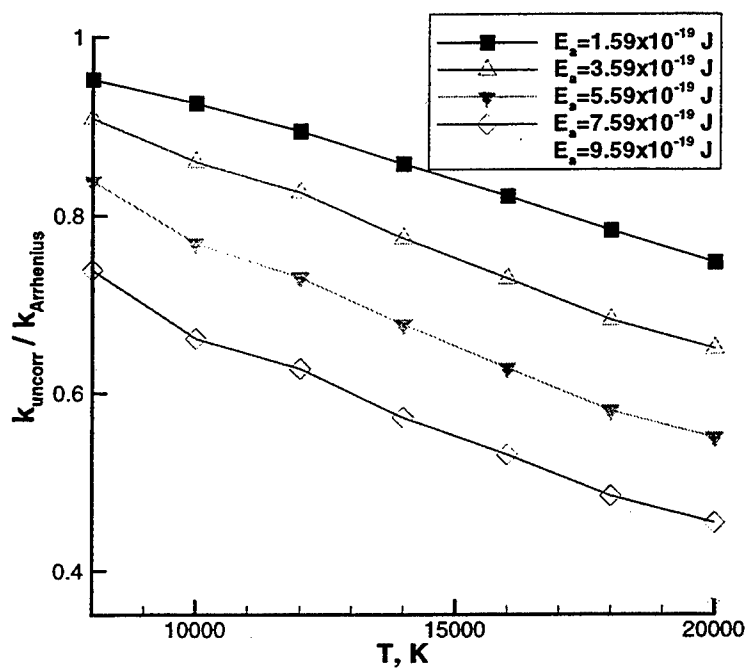


Figure 2: The impact of the parameter E_a in the Arrhenius fit on the ratio of the uncorrected to original reaction rate constants.

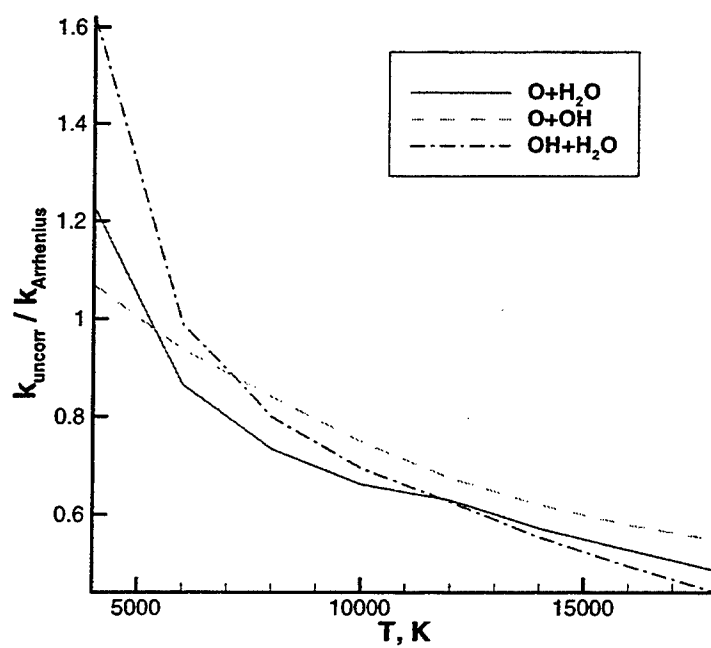


Figure 3: The impact of reactants on the ratio of the uncorrected to original reaction rate constants.

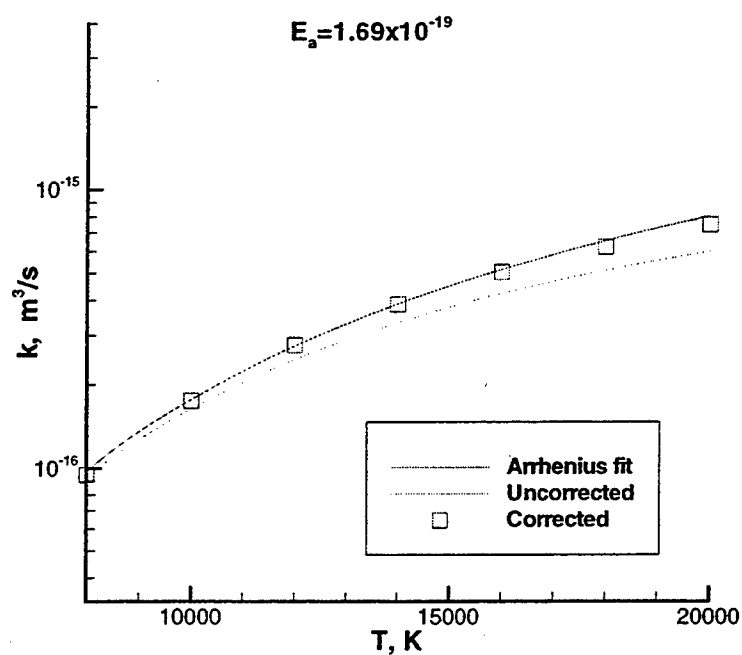


Figure 4: Corrected and uncorrected rates for $E_a = 1.69 \times 10^{-19}$ J.

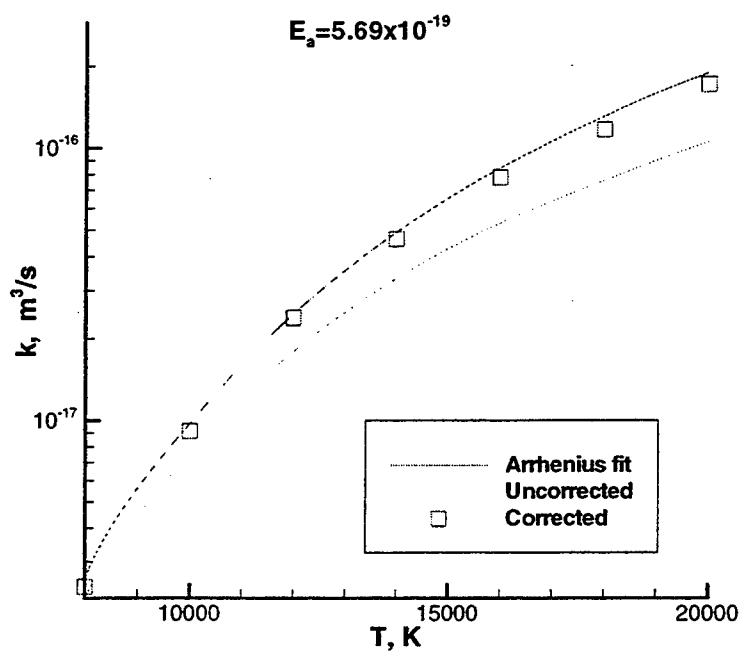


Figure 5: Corrected and uncorrected rates for $E_a = 5.69 \times 10^{-19}$ J.

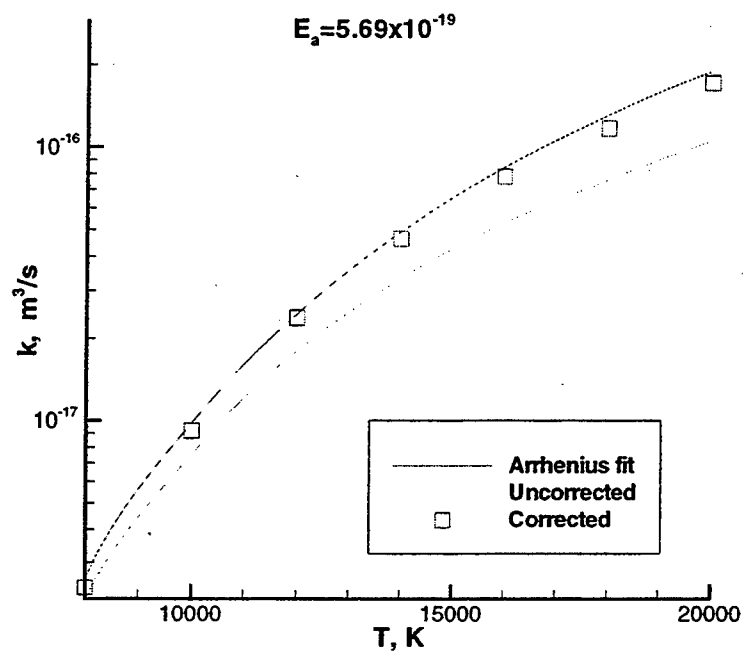


Figure 6: Corrected and uncorrected rates for $E_a = 9.69 \times 10^{-19}$ J.

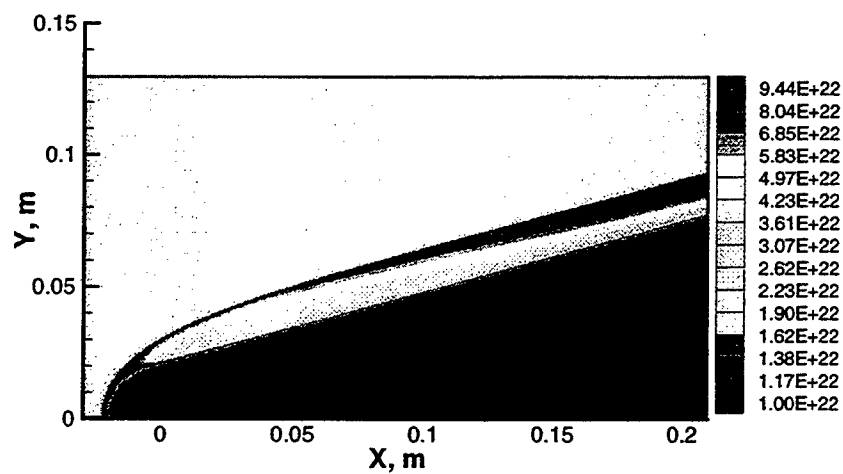


Figure 7: Total number density field about a rocket forebody.

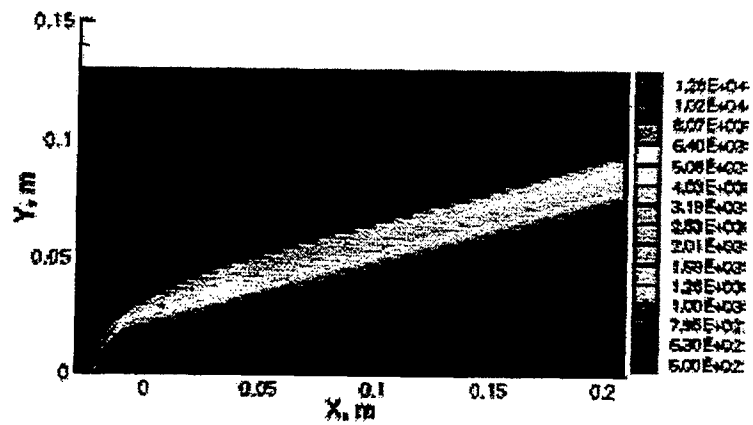


Figure 8: Translational temperature field about a rocket forebody.

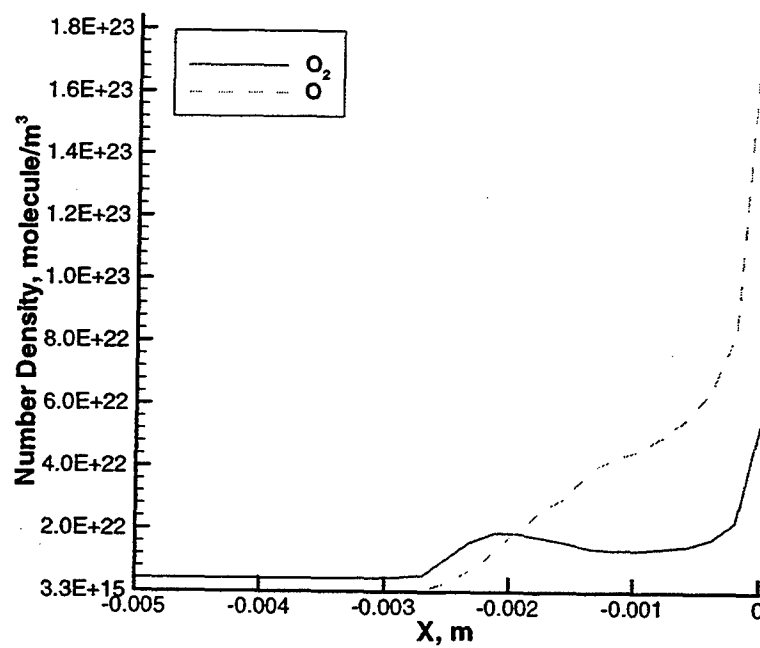


Figure 9: Total number density about a rocket forebody.

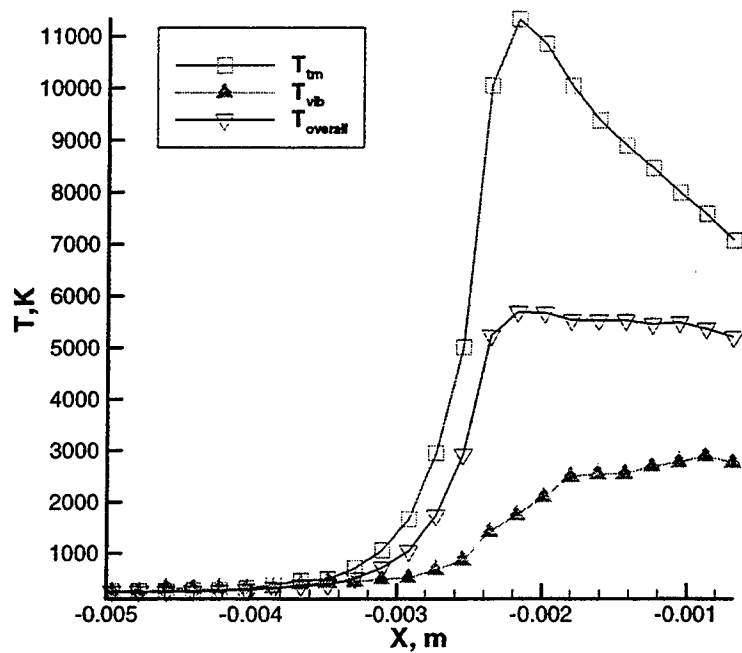


Figure 10: Comparison of different H₂O temperatures along the stagnation line.

Figure 11: Reaction rate constant as a function of temperature for different reactions.

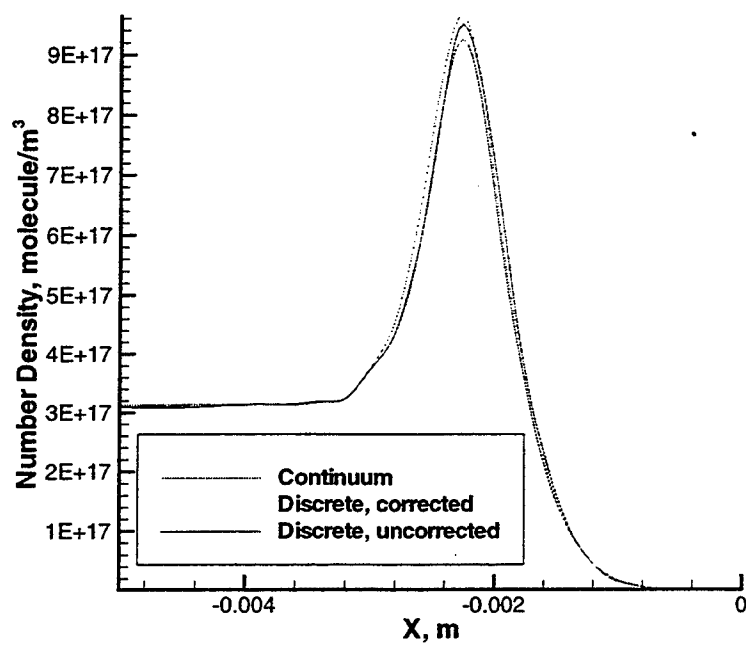


Figure 12: Comparison of H₂O number density profiles along the stagnation line for different models.

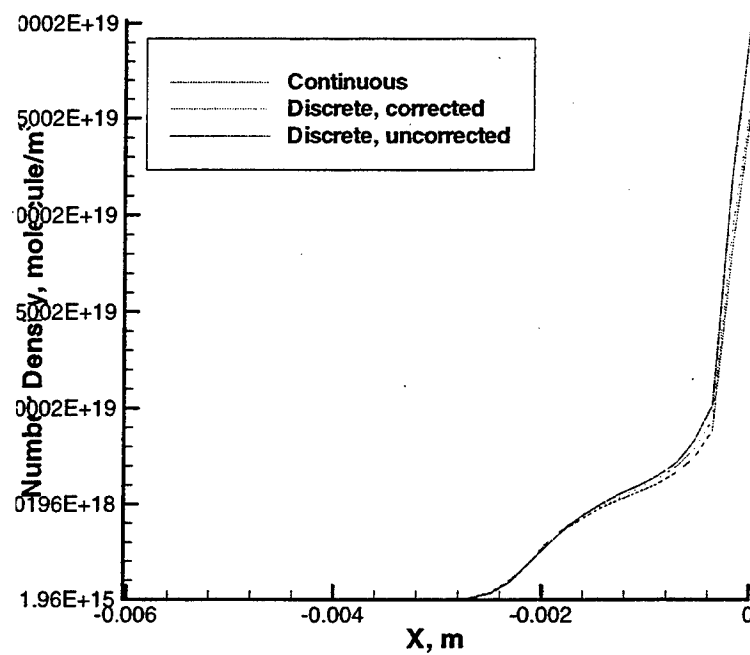


Figure 13: Comparison of OH number density profiles along the stagnation line for different models.

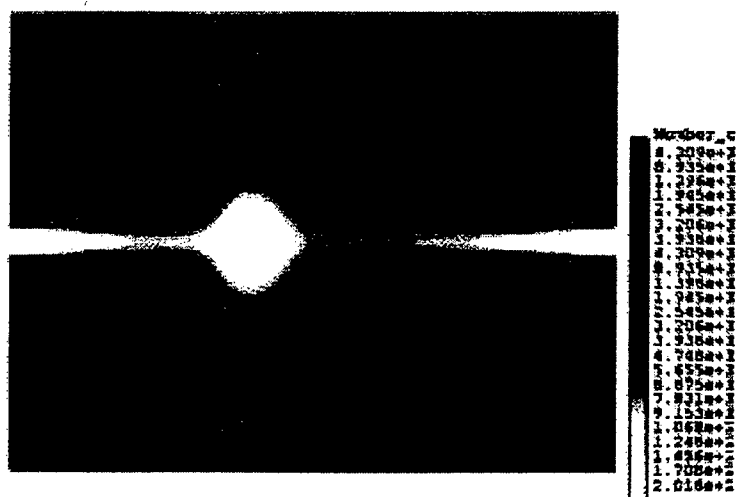


Figure 14: Total number density field for the counter plume flow.

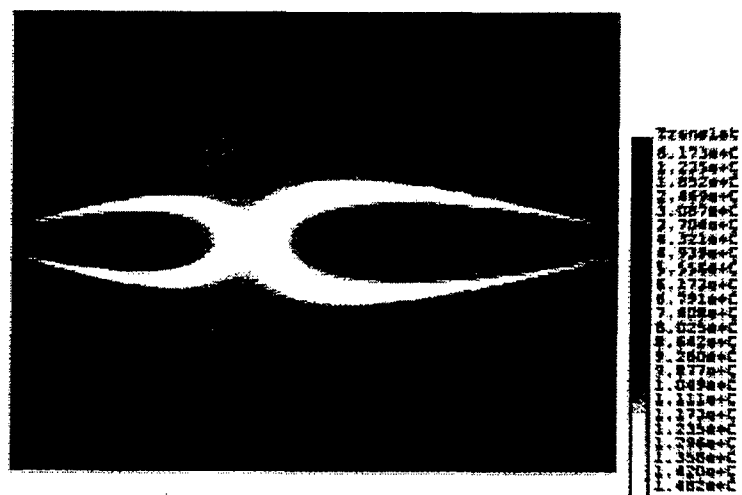


Figure 15: Translational temperature field for the counter plume flow.